

## lecture 3-1

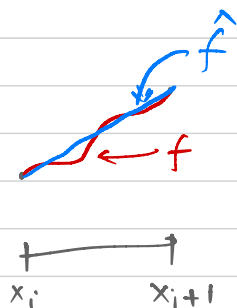
### Curve fitting & interpolation

- Curve fitting
  - linear regression
  - general linear regression
  - interpolation
  - Direct polynomial method
  - Newton's interpolation method
  - Lagrange's interpolation method
  - piecewise interpolation
- Integration
- Trapezoidal rule (linear interpolation)
  - Simpson's  $\frac{1}{2}$ nd rule (quadratic interpolation)
  - Simpson's  $\frac{3}{8}$ th rule (cubic interpolation)
  - Integration using general order polynomial interpolation
  - Error in numerical integration
  - Integration of functions

• Error in numerical integration

Trapezoidal rule

$$E_t^i = \int_{x_i}^{x_{i+1}} f(x) dx - \int_{x_i}^{x_{i+1}} \hat{f}(x) dx$$



$\hat{f}$  linear interpolation using

$$(x_i, f(x_i)), (x_{i+1}, f(x_{i+1}))$$

we can show

$$E_t^i = -\frac{(x_{i+1}-x_i)^3}{12} f^{(2)}(\xi_i)$$

$$f^{(k)}(x) = \frac{d^k f}{dx^k}$$

$$\therefore E_t = \sum_{i=1}^n E_t^i$$

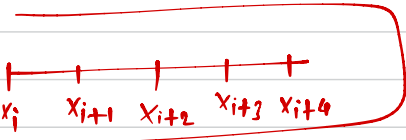
$$= -\frac{(b-a)^3}{12n^3} \sum_{i=1}^n f^{(2)}(\xi_i)$$

$$= -\frac{(b-a)^3}{12n^2} \bar{f}^{(2)}$$

assuming

$$x_{i+1} - x_i = h = \frac{(b-a)}{n}$$

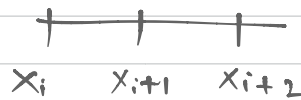
$$\bar{f}^{(k)} = \frac{1}{n} \sum_{i=1}^n f^{(k)}(\xi_i)$$



• Simpson's  $\frac{1}{3}$ rd rule (quadratic interpolation)

$$E_t^I = -\frac{1}{90} \left( \frac{x_{i+2} - x_i}{2} \right)^5 f^{(4)}(\xi_i)$$

$$= -\frac{h^5}{90} f^{(4)}(\xi_i)$$



assuming

$$x_{i+1} - x_i = \frac{b-a}{n} = h$$

even segment  
- odd points

$$I = 1 \rightarrow (x_1, x_3)$$

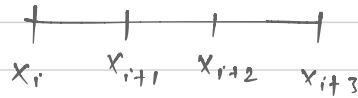
$$I = 2 \rightarrow (x_3, x_5)$$

⋮

$$I = m \rightarrow (x_{n-1}, x_{n+1})$$

sum  $E_t^I$  to get total error

• Simpson's  $\frac{3}{8}$ th rule



$$E_t^I = -\frac{3}{80} \left( \frac{x_{i+3} - x_i}{3} \right)^5 f^{(4)}(\xi)$$

$$= -\frac{3}{80} h^5 f^{(4)}(\xi)$$

$$\begin{aligned} x_{i+1} - x_i &= x_{i+2} - x_{i+1} \\ &= \dots = \frac{b-a}{n} \\ &= h \end{aligned}$$

$$I = 1 \rightarrow (x_1, x_4)$$

$$I = 2 \rightarrow (x_4, x_7)$$

⋮

## Integration of function

$$f: [a, b] \rightarrow (-\infty, \infty)$$

we can compute  $f$  at discrete points  $(x_1, x_2, \dots, x_n)$

$$(y_1 = f(x_1), y_2 = f(x_2), \dots, y_n = f(x_n))$$

Idea is to choose discrete points  $(x_1, x_2, \dots, x_n)$  more wisely to further reduce errors.

- Gauss Quadrature method
- Richardson's method
- Adaptive Quadrature

# Gauss quadrature method

## accurate upto linear functions

$$\hat{I}[f] = c_1 f(a) + c_2 f(b)$$

$$\bullet \quad I[1] = \hat{I}[1]$$

$$\Rightarrow c_1 + c_2 = \int_a^b 1 dx = b-a$$

$$\bullet \quad I[x] = \hat{I}[x]$$

$$\Rightarrow c_1 a + c_2 b = \int_a^b x dx = \frac{b^2 - a^2}{2}$$

$$f = \alpha + \beta x$$

$$I[f] = \hat{I}[f]$$

$$I[f] = \int_a^b (\alpha + \beta x) dx$$

$$= \alpha \int_a^b dx + \beta \int_a^b x dx$$

$$= \alpha I[1] + \beta I[x]$$

$$= \alpha \hat{I}[1] + \beta \hat{I}[x]$$

$$= \hat{I}[\alpha + \beta x]$$

Solve for  $c_1$  and  $c_2$

$$c_1 = c_2 = \frac{b-a}{2}$$

$$\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$$

find  $c_1, c_2, x_1, x_2$

$$\bullet \quad I[1] = \hat{I}[1]$$

$$\bullet \quad I[x] = \hat{I}[x]$$

$$\bullet \quad I[x^2] = \hat{I}[x^2]$$

$$\bullet \quad I[x^3] = \hat{I}[x^3]$$

Eq 1

$$c_1 + c_2 = b-a \Rightarrow c = \frac{b-a}{2}$$

Eq 2

$$c_1 x_1 + c_2 x_2 = \frac{b^2 - a^2}{2} \Rightarrow c(x_1 + x_2) = \frac{b^2 - a^2}{2}$$

$$\checkmark c(a+b) = \frac{b^2 - a^2}{2}$$

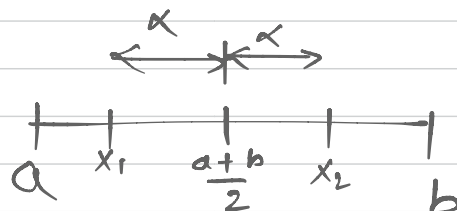
$$\Rightarrow c = \frac{b-a}{2}$$

Eq 3

$$c_1 x_1^2 + c_2 x_2^2 = \frac{b^3 - a^3}{3} \Rightarrow$$

Eq 4

$$c_1 x_1^3 + c_2 x_2^3 = \frac{b^4 - a^4}{4}$$



$$\bullet \quad c_1 = c_2 = c$$

$$\bullet \quad x_1 = \frac{(a+b)}{2} - \alpha$$

$$\bullet \quad x_2 = \frac{(a+b)}{2} + \alpha$$

$$C(x_1^2 + x_2^2) = \frac{b^3 - a^3}{3}$$

$$\rightarrow C\left(\left(\frac{a+b}{2} - \alpha\right)^2 + \left(\frac{a+b}{2} + \alpha\right)^2\right) = \frac{b^3 - a^3}{3}$$

$$\begin{aligned} \rightarrow \left(\frac{a+b}{2}\right)^2 + \alpha^2 - \cancel{(a+b)\alpha} + \left(\frac{a+b}{2}\right)^2 + \alpha^2 + \cancel{(a+b)\alpha} \\ = \frac{1}{c} \frac{(b^3 - a^3)}{3} \end{aligned}$$

$$\rightarrow 2\alpha^2 = \frac{1}{c} \frac{(b^3 - a^3)}{3} - 2 \frac{(a+b)^2}{2}$$

$\rightarrow$

•  $x_1, x_2$  are quadrature points

$$\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$$

$$c_1 = c_2 = \frac{b-a}{2}$$

$$x_1 = \frac{(a+b)}{2} - \alpha, \quad x_2 = \frac{(a+b)}{2} + \alpha$$

• Gauss-Legendre formula

$$f = \alpha_1 + \alpha_2 x + \alpha_3 x^2 + \alpha_4 x^3$$

$$\begin{aligned} I[f] &= \alpha_1 I[1] + \alpha_2 I[x] \\ &\quad + \alpha_3 I[x^2] \\ &\quad + \alpha_4 I[x^3] \end{aligned}$$

$$\begin{aligned} &= \alpha_1 \hat{I}[1] + \alpha_2 \hat{I}[x] \\ &\quad + \alpha_3 \hat{I}[x^2] \\ &\quad + \alpha_4 \hat{I}[x^3] \end{aligned}$$

$$= \hat{I}[\alpha_1 + \alpha_2 x + \alpha_3 x^2 + \alpha_4 x^3]$$

## Lecture 32

- Gauss Quadrature Method (Gauss-Legendre formulas)

for  $\hat{I}[f] = c_1 f(x_1) + c_2 f(x_2)$   $f: [a, b] \rightarrow (-\infty, \infty)$

find  $c_1, c_2, x_1, x_2$  s.t.

- $\hat{I}[1] = \hat{I}[1]$
- $\hat{I}[x] = \hat{I}[x]$
- $\hat{I}[x^2] = \hat{I}[x^2]$
- $\hat{I}[x^3] = \hat{I}[x^3]$

we found that

- $c_1 = c_2 = \frac{b-a}{2} = c$

- $x_1 = \frac{b+a}{2} - \alpha, \quad x_2 = \frac{b+a}{2} + \alpha$  where

$$2\alpha^2 = \frac{1}{c} \frac{(b^3 - a^3)}{3} - \frac{(a+b)^2}{2}$$

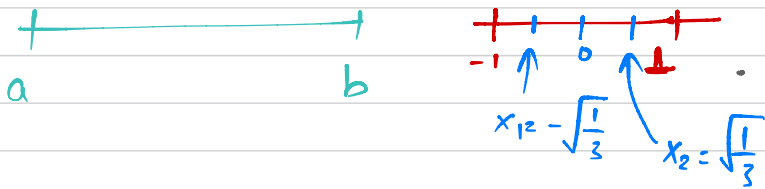
Take  $a = -1, b = 1$  then •  $c_1 = c_2 = 1 = c$

- $2\alpha^2 = \frac{1}{1} \frac{(1+1)}{3} - \frac{0^2}{2} = \frac{2}{3}$

$\Rightarrow \alpha = \sqrt{\frac{1}{3}}$

- $x_1 = \frac{b+a}{2} - \alpha = -\sqrt{\frac{1}{3}}$

- $x_2 = \frac{b+a}{2} + \alpha = \sqrt{\frac{1}{3}}$



$$\hat{I}[f] = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \quad \text{for } f: [-1, 1] \rightarrow (-\infty, \infty)$$

## Change of variable

let  $f: [a, b] \rightarrow (-\infty, \infty)$

$$I[f] = \int_a^b f(x) dx,$$

Consider

$$z = \alpha + \beta x$$

choose  $\alpha, \beta$  s.t.

$$\Rightarrow x = \frac{z - \alpha}{\beta}, \quad dx = \frac{dz}{\beta}$$

- $z = -1$  at  $x = a$

then

$$I[f] = \int_{-1}^1 f\left(\frac{z-\alpha}{\beta}\right) \frac{dz}{\beta}$$

$$= \frac{1}{\beta} \int_{-1}^1 f\left(\frac{z-\alpha}{\beta}\right) dz$$

define

$$g(z) = f\left(\frac{z-\alpha}{\beta}\right)$$

then

$$g: [-1, 1] \rightarrow (-\infty, \infty)$$

$$\therefore I[f] = \frac{1}{\beta} I[g]$$

$$= \frac{1}{\beta} \left( \int_{-1}^1 g(x) dx \right)$$

we quadrature formula that we obtained for

$$f: [-1, 1] \rightarrow (-\infty, \infty).$$

$$\hat{I}[g] = g\left(-\frac{1}{\sqrt{2}}\right) + g\left(\frac{1}{\sqrt{2}}\right)$$

Higher order formula

we can consider  $\hat{I}[f] = G_1 f(x_1) + G_2 f(x_2) + \dots + G_n f(x_n)$

which has  $2n$  unknowns so we can exactly

integrate upto  $(2n-1)^{th}$  order polynomial

$$\bullet I[1] = \hat{I}[1]$$

$$\bullet I[x] = \hat{I}[x]$$

$$\bullet z = 1 \text{ at } x = b$$

$$\frac{1}{\beta} \left. \begin{aligned} \alpha + \beta a &= -1 \\ \alpha + \beta b &= 1 \end{aligned} \right\}$$

$$\alpha + \beta b = 1$$

$$\beta(a-b) = -1-1$$

$$\Rightarrow \beta = \frac{2}{b-a}$$

$$\therefore \alpha = 1 - \frac{2}{b-a} b$$

$$\therefore z = \frac{b-a-2b}{b-a} + \frac{2}{b-a} x$$

$$\Rightarrow z = -\frac{(a+b)}{b-a} + \frac{2}{b-a} x$$

check

$$\text{when } x=a, \quad z = -\frac{(a+b)}{b-a} + \frac{2a}{b-a}$$

$$= \frac{1}{b-a} (2a - a - b)$$

$$= -1$$

$$\text{when } x=b, \quad z = 1.$$

$$\left. \begin{array}{l} \vdots \\ \cdot \end{array} \right\} \begin{array}{l} \\ \cdot \end{array} \left. \begin{array}{l} \\ \cdot \end{array} \right\} \rightarrow \text{an equation}$$

$$\cdot \mathbb{I}[x^{2n-1}] = \hat{\mathbb{I}}[x^{2n-1}]$$

Table 20.1 provides values of unknowns upto  $n=6$

### Richardson's Extrapolation

$$f: [a, b] \rightarrow (-\infty, \infty)$$

$$h_1 = \frac{b-a}{n_1-1}, \quad x_1 = a, \quad x_2 = x_1 + h_1, \quad x_3 = x_2 + h_1, \dots, \quad x_{n_1} = b$$

$$f(x_1), f(x_2), f(x_3), \dots, f(x_{n_1})$$

$$\mathbb{I}[f] = \int_a^b f(x) dx \approx \underbrace{\frac{h_1}{2} [f(x_1) + 2f(x_2) + \dots + f(x_{n_1})]}_{\hat{\mathbb{I}}[h_1]}$$

$$h_2 = \frac{b-a}{n_2-1}, \quad x_1 = a, \quad x_2 = x_1 + h_2, \quad x_3 = x_2 + h_2, \dots, \quad x_{n_2} = b$$

$$\mathbb{I}[f] = \int_a^b f(x) dx \approx \underbrace{\frac{h_2}{2} [f(x_1) + 2f(x_2) + \dots + 2f(x_{n_2-1}) + f(x_{n_2})]}_{\hat{\mathbb{I}}[h_2]}$$

In general we can write

$$\mathbb{I}[f] = \hat{\mathbb{I}}[h_1] + E[h_1], \quad \mathbb{I}[f] = \hat{\mathbb{I}}[h_2] + E[h_2]$$

$$\hat{\mathbb{I}}[h_1] + E[h_1] = \hat{\mathbb{I}}[h_2] + E[h_2]$$



for Trapezoidal rule,

$$E[h] = -\frac{(b-a)^2}{12} h^2 \bar{f}^{(2)}[h]$$

Assume that  $\bar{f}^{(2)}[h]$  is almost constant for different  $h$ .

$$\bar{f}^{(k)}[h] = \frac{1}{n} \sum_{i=1}^n f^{(k)}(z_i)$$

- $f^{(k)} = \frac{d^k f}{dx^k}$
- $h = \frac{b-a}{n-1}$

$$E[h_1] = -\frac{(b-a)^2}{12} h_1^2 \bar{f}^{(2)}[h_1]$$

$$E[h_2] = -\frac{(b-a)^2}{12} h_2^2 \bar{f}^{(2)}[h_2]$$

divide

$$\frac{E[h_1]}{E[h_2]} = \frac{h_1^2}{h_2^2} \frac{\bar{f}^{(2)}[h_1]}{\bar{f}^{(2)}[h_2]}$$

$$\Rightarrow \frac{E[h_1]}{E[h_2]} \approx \frac{h_1^2}{h_2^2}$$

Combine with  $\hat{I}[h_1] + E[h_1] = \hat{I}[h_2] + E[h_2]$

$$\Rightarrow \hat{I}[h_1] + E[h_2] \frac{h_1^2}{h_2^2} \stackrel{(\approx)}{=} \hat{I}[h_2] + E[h_2]$$

$$\Rightarrow E[h_2] \approx \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}}$$

$$I \approx \hat{I}[h_1] + \frac{\hat{I}[h_2] - \hat{I}[h_1]}{1 - h_1^2/h_2^2}$$

from  $I = \hat{I}[h_2] + E[h_2]$   $\nearrow$

$$I \approx \hat{I}[h_2] + \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - \frac{h_1^2}{h_2^2}}$$

Richardson's Extrapolation

$$\hat{I}[h] \rightarrow O(h^2)$$

$$E[h] = -\frac{(b-a)^2}{12} (h^2) f^{(2)}[h]$$

$$\hat{I}[h_2] + \frac{\hat{I}[h_1] - \hat{I}[h_2]}{1 - h_1^2/h_2^2} \rightarrow O(h_2^4)$$

Specific  $h_1 = h, h_2 = \frac{h}{2}$

$$I \approx \hat{I}[h/2] + \frac{\hat{I}[h] - \hat{I}[h/2]}{1 - \frac{h^2}{h^2/4}} \rightarrow 1 - 4$$

$$= \hat{I}[h/2] - \frac{1}{3} (\hat{I}[h] - \hat{I}[h/2])$$

$$= \hat{I}[h/2] \left(1 + \frac{1}{3}\right) - \frac{1}{3} \hat{I}[h]$$

$$\Rightarrow I \approx \frac{4}{3} \hat{I}[h/2] - \frac{1}{3} \hat{I}[h]$$